

REMARKS/ARGUMENTS

Favorable reconsideration of this application as presently amended and in light of the following discussion is respectfully requested.

Claims 1-48 are pending in the present application. Claims 1, 3-5, 13, 15-18, 28, 31, 33, 34, 36, 37, and 47 are amended by the present amendment.

In the outstanding Office Action, Claims 1-4, 10, 13, 15-17, 23, 26, 28-31, 33-37, 40, 44, and 46-48 were rejected under 35 U.S.C. § 102(b) as anticipated by Wade et al. ("Development of Algorithms for Automated Elucidation of Spectral Feature/Substructure Relationships in Tandem Mass Spectrometry," *Analytica Chimica Acta*, 215 (1988) 169-186, herein "Wade"); Claims 1-2, 10, 12-13, 28-31, 33-35, 37, 40, 43-44, and 46-48 were rejected under 35 U.S.C. § 102(b) as anticipated by Kwiatkowski ("A Combined Forward-Reverse Library Search System for Identification of Low-Resolution Mass Spectra," *Aalytica Chimica Acta*, 112 (1979) 219-231, herein "Kwiatkowski"); Claims 1-4, 10, 13, 15-17, 23, 26, 28-31, 33-37, 40, 44, and 46-48 were rejected under 35 U.S.C. § 103(a) as unpatentable over Wade in view of Amado (U.S. Patent No. 5,701,400), Eisenberg (U.S. Patent No. 6,453,242) and Yates (U.S. Patent No. 6,017,693); Claims 1, 2, 10, 12, 13, 28-31, 33-35, 37, 40, 43, 44, and 46-48 were rejected under 35 U.S.C. § 103(a) as being unpatentable over Kwiatkowski in view of Amado, Eisenberg, and Yates; and Claims 5-9, 11, 14, 18-22, 24, 25, 27, 32, 38, 39, 41, 42, and 45 were indicated as allowable if rewritten in independent form.

Applicants thank the Examiner for the indication of allowable subject matter. However, in view of the amendment to the independent claims, the allowed claims are maintained in dependent form.

Applicants also thank the Examiner for the courtesy of an interview extended to Applicants' representative on Tuesday 12, 2006. During the interview, the differences between the claims and the applied art were discussed. Further, clarifying claim

amendments, similar to those presented herewith, were also discussed. The Examiner indicated he would further review the amended claims in view of a filed response.

Arguments presented during the interview are reiterated below.

Regarding the rejections on the merits of the independent claims, each independent claim has been amended to more clearly recite that a mass spectrum is mined based on primary spectral characteristics and secondary spectral characteristics associated with respective of the primary spectral characteristics, and the secondary spectral characteristics are used to search the mass spectrum when matching portions of the mass spectrum are found to match the primary spectral characteristics. The claim amendments find support in the specification, for example at page 12, line 22, to page 13, line 14. No new matter has been added.

Briefly recapitulating, independent Claim 1 is directed to a method for mining a mass spectrum based on arbitrarily selected primary and secondary spectral characteristics input by a user. The secondary spectral characteristics are associated with respective of the primary spectral characteristics. The method recites, *inter alia*, searching the mass spectrum for a matching portion which matches the primary spectral characteristics, and, when a match is found, searching the matching portion of the mass spectrum for subportions that match the secondary spectral characteristics associated with the primary spectral characteristics for which the match was found.

As discussed in the specification at page 7, line 27 to page 8, line 9, conventional mining mass spectrum methods are able to identify known chemical species that are found in the mass spectrum to be mined based on predetermined patterns stored in a library. However, as also disclosed in the same paragraph of the specification, there are many unanticipated modifications of the given chemical species and thus, the size of the library is large and a conventional search of the entire library is slow and impractical.

In addition, the conventional methods search and compare an unknown mass spectrum with spectral characteristics that fully define respective known compounds. In other words, detailed spectral characteristics of known compounds are correlated with the unknown mass spectrum. Thus, the conventional search is limited to searching known detailed spectral patterns peculiar only to the specific respective compound. The conventional search is only useful for identifying the known compound when a match occurs. Also, the conventional methods need to use one full set of spectral characteristics to identify the known compound because that set fully characterizes the compound. Further, the specification explains at page 2, lines 25-32, other limitations with which the conventional methods are faced.

On the contrary, the claimed method permits a search of a compound in a mass spectrum based on input spectral characteristics that may be independent of the specific knowledge compound. In other words, the input spectral characteristics may be less than a full set of spectral characteristics that define the compound. Thus, the claimed method does not rely on a library of stored know compounds, and therefore, the speed of the search is not slowed down by the size of the library, which is usually large.

Further, the claimed method performs searching in stages. First, an initial search based on the primary spectral characteristics is performed to identify portions of the spectrum that match the primary spectral characteristics. When a match has occurred for the primary spectral characteristics, a secondary search is only then performed for the secondary spectral characteristics associated with the primary spectral characteristics for which the match was found. If no match of primary spectral characteristics is found, secondary searching is not performed.

Thus, the claimed method has among other advantages, the capability to select desired spectral characteristics that are independent of the patterns existing in preexisting libraries,

and to more efficiently perform the search based on a reduced number of spectral characteristics.

Turning to the applied art, Wade teaches a MAPS algorithm that uses relationships that exist between substructures in molecules and characteristic features they produce in mass spectroscopy, as recognized in the outstanding Office Action at page 2, numbered paragraph 4. Wade specifically discloses at page 170, second full paragraph, that the computer method “automatically searches for and identifies spectral feature/substructure relationships from experimental spectra by applying **basic chemical principles** and **pattern recognition techniques**.” Further, at page 174, first full paragraph, Wade discloses that a training set is generated based on data from **known** compounds. Furthermore, Wade discloses at page 176, second full paragraph, that “each spectral feature in each rule has some level of correlation with the substructure.” In other words, Wade relies on preexisting known compounds based on which various rules are determined and use those rules to search the mass spectrum. However, Wade does not teach or suggest first searching the mass spectrum based on primary spectral characteristics, and when a match of the primary spectral characteristics is found, then searching the mass spectrum based on the secondary spectral characteristics.

On the contrary, Wade searches the mass spectrum based on all available spectral characteristics without discriminating between primary and secondary spectral characteristics and without associating respective secondary spectral characteristics to primary spectral characteristics.

Kwiatkowski discloses a forward/reverse library search system and a method that relies on library stored spectra for identifying compounds identical to those already stored in the library, which is similar to Wade. However, Kwiatkowski does not teach or suggest first searching the mass spectrum based on primary spectral characteristics, and when a match of

the primary spectral characteristics is found, then searching the mass spectrum based on the secondary spectral characteristics, as required by amended Claims 1, 15, 28, 33, 34, and 47.

Amado, Eisenberg, and Yates have been considered but do not cure the deficiencies of Wade and Kwiatkowski discussed above with regard to independent Claims 1, 15, 28, 33, 34, and 47. Accordingly, it is respectfully submitted that independent Claims 1, 15, 28, 33, 34, and 47 and each of the claims depending therefrom patentably distinguish over Wade, Kwiatkowski, Amado, Eisenberg, and Yates, either alone or in any combination.

Consequently, in light of the above discussion and in view of the present amendment, the present application is believed to be in condition for allowance and an early and favorable action to that effect is respectfully requested.

Respectfully submitted,

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